

10584017.txt

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(FILE 'HOME' ENTERED AT 21:38:24 ON 06 JAN 2008)

FILE 'REGISTRY' ENTERED AT 21:38:55 ON 06 JAN 2008

L1           STRUCTURE UPLOADED

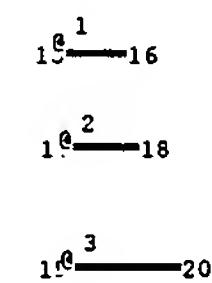
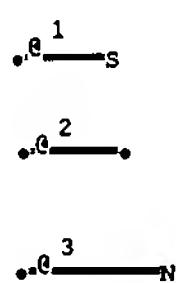
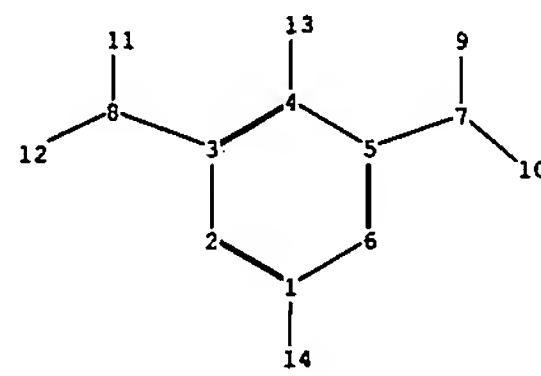
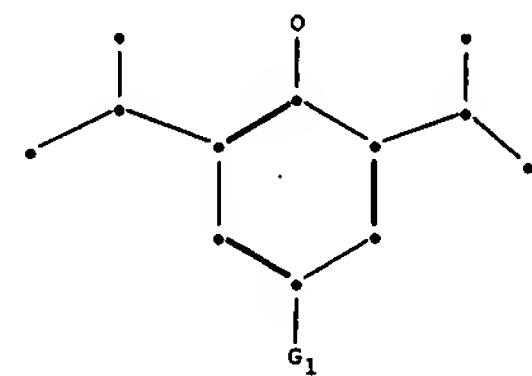
L2           50 S L1

L3           3801 S L1 FULL

FILE 'HCAPLUS, CHEMCATS' ENTERED AT 21:41:16 ON 06 JAN 2008

L4           3722 S L3

L5           14 S L4 AND (PROPOFOL OR DIISOPROPYLPHENOL)



chain nodes :

7 8 9 10 11 12 13 14 15 16 17 18 19 20

ring nodes :

1 2 3 4 5 6

chain bonds :

1-14 3-8 4-13 5-7 7-9 7-10 8-11 8-12 15-16 17-18 19-20

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

1-14 4-13 15-16 19-20

exact bonds :

3-8 5-7 7-9 7-10 8-11 8-12 17-18

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

G1:[\*1],[\*2],[\*3]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS8:CLASS9:CLASS10:CLASS11:CLASS12:CLASS13:CLASS14:CLASS15:CLASS16:CLASS17:CLASS18:CLASS19:CLASS20:CLASS